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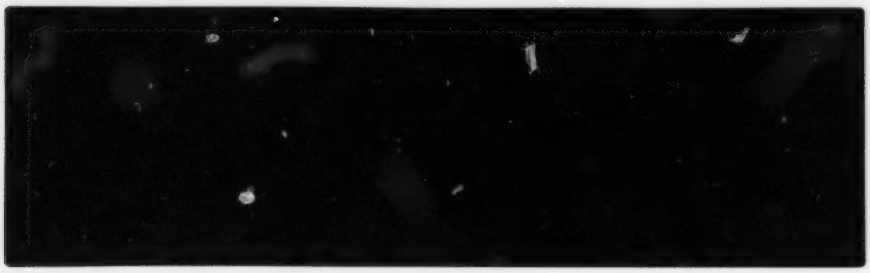

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CALCULATION OF THE REDUCED SECOND VIRIAL COEFFICIENT AND ITS DERIVATIVES

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CALCULATION OF THE REDUCED SECOND VIRIAL COEFFICIENT AND ITS DERIVATIVES

by

D.E.G. JONES*

SUMMARY

For n-m potential functions, improved analytical expressions for the reduced second virial coefficient, B^* and its first, B_1^* and second, B_2^* derivatives have been obtained, resulting in improved accuracy in values tabulated for a series of $T^*=kT/\varepsilon$, where k is the Boltzmann constant and ε, is the depth of the potential function well. Numerical techniques have been described and used to calculate the above values with consistent results.

These techniques have been extended to calculate the same values for the exp-6 potential function. Significantly more accurate values of both B^* and B_1^* than have been previously reported, have been obtained and additionally, the only known values of B_2^* have been determined.

All the thermodynamic functions characteristic of a given potential function may be estimated from the above information.

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KEYWORDS:

Second, virial, coefficient exp-6, potential, function derivatives, reduced, second, virial, coefficient TIGER, code numerical, differentiation, integration potential, function, parameters.

CALCUL DU SECOND COEFFICIENT VIRIEL RÉDUIT ET DE SES DÉRIVÉES

par

D.E.G. JONES*

SOMMAIRE

Pour les fonctions potentiel n-m, on a établi des expressions analytiques améliorées permettant de calculer le second coefficient viriel réduit, B* et ses dérivés première, B_1*, et seconde, B_2*, ce qui conduit à une plus grande précision des valeurs calculées pour une série T*=kTε, où k est la constante de Boltzmann et ε, la hauteur du puits de fonction potentiel. Les techniques numériques sont décrites et elles ont été utilisées pour calculer les valeurs ci-dessus, avec des résultats cohérents.

Ces techniques ont été perfectionnées pour calculer les mêmes valeurs de la fonction potentiel exp-6. On a ainsi obtenu des valeurs de B* et B_1* beaucoup plus précises que celles obtenues auparavant et, en outre, on a pu déterminer les seules valeurs connue de B_2*.

Les calculs ci-dessus permettent d'évaluer toutes les fonctions thermodynamiques caractéristiques d'une fonction potentiel donnée.

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MOTS CLÉS:

Second, viriel, coefficient exp-6, potentiel, dérivés d'une fonction, réduit, second, viriel, coefficient, TIGRE, code, numérique, différentiation, intégration, fonction potentiel, paramètres.

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INTRODUCTION

In an earlier report(1) an analytical expression for the reduced second virial coefficient, B^* for n-m potential functions, was obtained. This expression was used to calculate B^* for the 12.0-6.0 potential function and the results were compared with values determined numerically. The numerical method was found to give reliable results and was subsequently used to determine B^* for the exp-6 potential function.

B^* values can be used to determine the potential function parameters, ε/k and σ for a given equation of state used in the TIGER code, by comparison with experimental values of the second virial coefficient, B(T). The parameters ε/k and σ are, respectively, the depth of the potential well and the value of the intermolecular distance at which the potential energy vanishes.

The TIGER code is useful for estimating the explosion and detonation parameters for explosive substances and/or mixtures. It is necessary to have a reliable numerical technique to estimate ε/k and σ for use in this code. These parameters are essential in the use of the code as a predictive tool for classification of explosives with regard to fume composition on detonation and subsequent expansion.

Further, thermodynamic functions required in the code may be calculated from B^* and the derivatives T^*dB^*/dT^* (B_1^*) and $T^{*2}d^2B^*/dT^{*2}$ (B_2^*), where $T^*=kT/\varepsilon(3)$.

It is the purpose of this report to demonstrate numerical techniques for calculating B^*, B_1^* and B_2^*. Tables of the most accurate values of B^* and B_1^* yet presented and the first values of B_2^* ever presented, will be given for the exp-6 function.

n-m POTENTIAL FUNCTIONS

1. Analytical Results

A. The Reduced Second Virial Coefficient B^*

The analytical expression for B^* for a n-m potential function,

$$U(r) = f(n,m)\,\varepsilon\,[(\sigma/r)^n - (\sigma/r)^m] \qquad [1]$$

where r is the intermolecular separation and
$f(n,m) = (n/m)^{m/(n-m)}\; n/(n-m)$, is obtained by integrating,

$$B(T) = (2\pi N_A/3kT)\int_0^\infty r^3[dU(r)/dr]\exp(-U(r)/kT)dr \qquad [2]$$

The result is

$$B^* = \sum_j [a^{j-f_2}\Gamma(f_2)]/(j-1)! - (m/n)\sum_j [a^{j-f_1}\Gamma(f_1)]/(j-1)! \qquad [3]$$

where $a = f(n,m)/T^*$, $f_1 = (jm-3)$,

$f_2 = [n+(j-1)m-3]/n$ and

$$\Gamma(x) = b^x\int_0^\infty t^{x-1}e^{-bt}dt \qquad [4]$$

Since $\Gamma(x)$ can be calculated accurately by standard subroutines(2), B^* can easily be calculated from [3], for given values of T^*, n and m.

In practice, the factorial terms in [3] determine the accuracy limits in the calculation of B^*. These limits are dependant on the floating point precision of the computer used. Tables 1, 2 and 3 list values of B^* calculated from [3] for a series of T^* for the 9.0-6.0, 12.0-6.0 and 15.0-6.0 potential functions. The column under the heading DIFF in these Tables represents the difference between successive values of B^* at which the summation in [3] is stopped.

The program used to calculate the values in Tables 1 to 3 is listed in Apendix A.

Table 1 - Reduced 2nd Virial Coefficient Parameters
for the 9.0 - 6.0 Potential Function

T*	B*	B_1*	B_2*	J	Diff
.75	-5.5106633609	9.09797258	-25.761541	47	.75E-10
.80	-4.9565058549	8.09994538	-22.438061	46	.64E-10
.85	-4.4906338151	7.28752758	-19.803267	45	.60E-10
.90	-4.0937104734	6.61488339	-17.673418	44	.60E-10
.95	-3.7516270600	6.04979972	-15.922732	43	.66E-10
1.00	-3.4538570111	5.56905543	-14.462714	42	.77E-10
1.05	-3.1923922522	5.15553632	-13.229595	42	.39E-10
1.10	-2.9610357057	4.79638080	-12.176447	41	.51E-10
1.15	-2.7549187104	4.48175476	-11.268084	40	.70E-10
1.20	-2.5701644176	4.20402230	-10.477680	40	.40E-10
1.25	-2.4036482784	3.95717192	-9.784478	39	.59E-10
1.30	-2.2528245415	3.73641168	-9.172195	39	.36E-10
1.35	-2.1155985260	3.53787853	-8.627905	38	.57E-10
1.40	-1.9902312053	3.35842617	-8.141229	38	.36E-10
1.45	-1.8752669751	3.19546796	-7.703751	37	.61E-10
1.50	-1.7694783014	3.04685906	-7.308581	37	.41E-10
1.55	-1.6718228291	2.91080692	-6.950030	36	.72E-10
1.60	-1.5814098004	2.78580246	-6.623366	36	.50E-10
1.65	-1.4974735155	2.67056667	-6.324622	36	.34E-10
1.70	-1.4193521690	2.56400877	-6.050449	35	.66E-10
1.75	-1.3464708387	2.46519309	-5.798003	35	.47E-10
1.80	-1.2783277054	2.37331266	-5.564857	35	.34E-10
1.85	-1.2144828118	2.28766796	-5.348925	34	.68E-10
1.90	-1.1545488306	2.20764981	-5.148404	34	.51E-10
1.95	-1.0981834368	2.13272525	-4.961735	34	.38E-10
2.00	-1.0450829668	2.06242614	-4.787554	34	.29E-10
2.10	-.9476245053	1.93410023	-4.472040	33	.47E-10
2.20	-.8603359904	1.81989970	-4.193946	33	.29E-10
2.30	-.7817352094	1.71762426	-3.947076	32	.51E-10
2.40	-.7106134277	1.62550599	-3.726514	32	.33E-10
2.50	-.6459751955	1.54210862	-3.528316	31	.63E-10
2.60	-.5869933679	1.46625347	-3.349278	31	.43E-10
2.70	-.5329750395	1.39696443	-3.186778	31	.29E-10
2.80	-.4833354221	1.33342638	-3.038644	30	.61E-10
2.90	-.4375775895	1.27495338	-2.903069	30	.43E-10
3.00	-.3952766073	1.22096416	-2.778531	30	.31E-10
3.10	-.3560669786	1.17096294	-2.663745	29	.69E-10
3.20	-.3196326266	1.12452428	-2.557615	29	.51E-10
3.30	-.2856988349	1.08128108	-2.459204	29	.38E-10
3.40	-.2540257128	1.04091492	-2.367704	29	.29E-10
3.50	-.2244028615	1.00314830	-2.282414	28	.70E-10
3.60	-.1966449886	.96773823	-2.202726	28	.54E-10

Table 1 - Reduced 2nd Virial Coefficient Parameters
for the 9.0 - 6.0 Potential Function (Cont'd)

T*	B*	B_1*	B_2*	J	Diff
3.70	-.1705882836	.93447107	-2.128108	28	.42E-10
3.80	-.1460874013	.90315822	-2.058093	28	.33E-10
3.90	-.1230129396	.87363258	-1.992269	28	.26E-10
4.00	-.1012493192	.84574554	-1.930271	27	.68E-10
4.10	-.0806929918	.81936454	-1.871777	27	.55E-10
4.20	-.0612509206	.79437091	-1.816498	27	.44E-10
4.30	-.0428392843	.77065816	-1.764178	27	.36E-10
4.40	-.0253823679	.74813039	-1.714584	27	.29E-10
4.50	-.0088116100	.72670105	-1.667510	27	.24E-10
4.60	.0069352190	.70629184	-1.622768	26	.67E-10
4.70	.0219147284	.68683170	-1.580191	26	.56E-10
4.80	.0361785244	.66825603	-1.539624	26	.47E-10
4.90	.0497737487	.65050598	-1.500928	26	.39E-10
5.00	.0627435486	.63352779	-1.463979	26	.33E-10
6.00	.1653758031	.49711453	-1.169280	25	.26E-10
7.00	.2344687772	.40209403	-.966196	24	.28E-10
8.00	.2833744972	.33214985	-.817751	23	.38E-10
9.00	.3192704524	.27854724	-.704508	22	.64E-10
10.00	.3463434234	.23618676	-.615275	22	.30E-10
20.00	.4383549293	.05251896	-.228535	19	.27E-10
30.00	.4471678697	-.00462595	-.105751	17	.66E-10
40.00	.4417531491	-.03145332	-.046246	16	.80E-10
50.00	.4329719226	-.04652282	-.011570	16	.25E-10
60.00	.4236000563	-.05588585	.010873	15	.64E-10
70.00	.4144868511	-.06208583	.026418	15	.30E-10
80.00	.4059019735	-.06637042	.037708	15	.15E-10
90.00	.3978988115	-.06941945	.046200	14	.65E-10
100.00	.3904641233	-.07163279	.052760	14	.40E-10
200.00	.3381074307	-.07722932	.077615	13	.16E-10
300.00	.3070108780	-.07575026	.082183	12	.29E-10
400.00	.2855272189	-.07347308	.082697	12	.93E-11

$B_1^* = T^* dB^*/dT^*$ $B_2^* = T^{*2} d^2B^*/dT^{*2}$

Table 2 - Reduced 2nd Virial Coefficient Parameters
for the 12.0 - 6.0 Potential Function

T*	B*	B_1*	B_2*	J	Diff
.30	-27.8805827612	76.60726271	-356.876821	48	.72E-10
.35	-18.7548949582	45.24771634	-189.465372	45	.43E-10
.40	-13.7988347194	30.26708015	-116.366036	42	.57E-10
.45	-10.7549741346	21.98948102	-78.877947	40	.46E-10
.50	-8.7202054245	16.92369146	-57.339522	38	.56E-10
.55	-7.2740854079	13.58215474	-43.882440	37	.30E-10
.60	-6.1979710553	11.24884992	-34.918688	35	.66E-10
.65	-5.3681917219	9.54550958	-28.640504	34	.56E-10
.70	-4.7100373167	8.25711511	-24.062665	33	.55E-10
.75	-4.1759282475	7.25401320	-20.613105	32	.63E-10
.80	-3.7342253581	6.45413992	-17.941897	32	.23E-10
.85	-3.3631194549	5.80340624	-15.825459	31	.32E-10
.90	-3.0471142840	5.26491820	-14.115570	30	.50E-10
.95	-2.7749102012	4.81276059	-12.710810	30	.23E-10
1.00	-2.5380813368	4.42826152	-11.539854	29	.41E-10
1.05	-2.3302211072	4.09766617	-10.551326	28	.78E-10
1.10	-2.1463741926	3.81064221	-9.707435	28	.42E-10
1.15	-1.9826492896	3.55929289	-8.979855	28	.23E-10
1.20	-1.8359491323	3.33748906	-8.347000	27	.51E-10
1.25	-1.7037784776	3.14040735	-7.792171	27	.30E-10
1.30	-1.5841050706	2.96420436	-7.302275	26	.73E-10
1.35	-1.4752573328	2.80578277	-6.866921	26	.46E-10
1.40	-1.3758479637	2.66262082	-6.477768	26	.29E-10
1.45	-1.2847161259	2.53264597	-6.128055	25	.78E-10
1.50	-1.2008831571	2.41414021	-5.812247	25	.52E-10
1.55	-1.1235182639	2.30566814	-5.525779	25	.35E-10
1.60	-1.0519116708	2.20602168	-5.264851	25	.24E-10
1.65	-.9854534051	2.11417722	-5.026279	24	.73E-10
1.70	-.9236163857	2.02926202	-4.807378	24	.51E-10
1.75	-.8659428331	1.95052761	-4.605866	24	.37E-10
1.80	-.8120332633	1.87732864	-4.419797	24	.26E-10
1.85	-.7615375123	1.80910584	-4.247497	24	.19E-10
1.90	-.7141473663	1.74537221	-4.087525	23	.66E-10
1.95	-.6695904741	1.68570185	-3.938628	23	.49E-10
2.00	-.6276252883	1.62972068	-3.799716	23	.37E-10
2.10	-.5506331761	1.52754451	-3.548144	23	.22E-10
2.20	-.4817100431	1.43662950	-3.326472	22	.63E-10
2.30	-.4196777384	1.35521892	-3.129740	22	.39E-10
2.40	-.3635757755	1.28190173	-2.954014	22	.25E-10
2.50	-.3126133703	1.21553191	-2.796139	22	.16E-10
2.60	-.2661336139	1.15516926	-2.653555	21	.55E-10
2.70	-.2235863461	1.10003535	-2.524164	21	.38E-10

Table 2 - Reduced 2nd Virial Coefficient Parameters for the 12.0 - 6.0 Potential Function (Cont'd)

T*	B*	B_1*	B_2*	J	Diff
2.80	-.1845073616	1.04948029	-2.406232	21	.26E-10
2.90	-.1485022890	1.00295732	-2.298314	21	.18E-10
3.00	-.1152339640	.96000321	-2.199195	20	.71E-10
3.10	-.0844124436	.92022289	-2.107850	20	.51E-10
3.20	-.0557870389	.88327748	-2.023402	20	.38E-10
3.30	-.0291399069	.84887455	-1.945105	20	.28E-10
3.40	-.0042808561	.81676055	-1.872313	20	.21E-10
3.50	.0189568930	.78671449	-1.804467	20	.16E-10
3.60	.0407201925	.75854292	-1.741083	19	.71E-10
3.70	.0611388474	.73207578	-1.681735	19	.55E-10
3.80	.0803280110	.70716296	-1.626052	19	.43E-10
3.90	.0983901887	.68367145	-1.573706	19	.34E-10
4.00	.1154169217	.66148301	-1.524405	19	.27E-10
4.10	.1314902092	.64049216	-1.477892	19	.22E-10
4.20	.1466837153	.62060448	-1.433937	19	.17E-10
4.30	.1610637976	.60173526	-1.392337	19	.14E-10
4.40	.1746903868	.58380820	-1.352906	18	.71E-10
4.50	.1876177441	.56675448	-1.315479	18	.58E-10
4.60	.1998951116	.55051180	-1.279908	18	.48E-10
4.70	.2115672780	.53502366	-1.246058	18	.40E-10
4.80	.2226750678	.52023868	-1.213807	18	.33E-10
4.90	.2332557683	.50611007	-1.183045	18	.28E-10
5.00	.2433435027	.49259507	-1.153670	18	.23E-10
6.00	.3229043726	.38397221	-.919393	17	.34E-10
7.00	.3760884670	.30825657	-.757930	16	.72E-10
8.00	.4134339538	.25248008	-.639879	16	.26E-10
9.00	.4405978375	.20970115	-.549792	16	.10E-10
10.00	.4608752839	.17586702	-.478779	15	.40E-10
20.00	.5253742041	.02866377	-.170403	13	.37E-10
30.00	.5269254583	-.01749286	-.072012	12	.40E-10
40.00	.5185750150	-.03931154	-.024109	12	.77E-11
50.00	.5083614319	-.05164776	.003927	11	.35E-10
60.00	.4982126049	-.05936206	.022147	11	.14E-10
70.00	.4886506891	-.06450394	.034817	11	.61E-11
80.00	.4797900961	-.06808188	.044055	10	.61E-10
90.00	.4716150439	-.07064701	.051031	10	.35E-10
100.00	.4640694689	-.07252443	.056441	10	.21E-10
200.00	.4114316789	-.07753999	.077296	9	.24E-10
300.00	.3801278828	-.07652453	.081397	9	.43E-11
400.00	.3583511814	-.07475339	.082055	8	.51E-10

$B_1^* = T^* dB^*/dT^*$ $\quad B_2^* = T^{*2} d^2B^*/dT^{*2}$

Table 3 - Reduced 2nd Virial Coefficient Parameters for the 15.0 - 6.0 Potential Function

T*	B*	B_1*	B_2*	J	Diff
.25	-41.2891161426	136.02190173	-725.354729	45	.27E-10
.30	-23.8378334415	65.79973132	-306.379858	41	.28E-10
.35	-15.9982589981	38.87888025	-162.697380	38	.30E-10
.40	-11.7390930332	26.01602888	-99.951909	35	.74E-10
.45	-9.1223495615	18.90710281	-67.769463	34	.25E-10
.50	-7.3725640583	14.55558941	-49.276756	32	.47E-10
.55	-6.1286438940	11.68459985	-37.720943	31	.32E-10
.60	-5.2027715085	9.67945264	-30.022492	30	.27E-10
.65	-4.4886905930	8.21538192	-24.629731	29	.29E-10
.70	-3.9221986437	7.10776042	-20.696943	28	.36E-10
.75	-3.4624002705	6.24524788	-17.733032	27	.52E-10
.80	-3.0820963149	5.55736359	-15.437575	27	.19E-10
.85	-2.7625349766	4.99764794	-13.618608	26	.34E-10
.90	-2.4903902872	4.53440742	-12.148859	25	.69E-10
.95	-2.2559436959	4.14537734	-10.941236	25	.31E-10
1.00	-2.0519472997	3.81451428	-9.934485	24	.74E-10
1.05	-1.8728894516	3.52999846	-9.084483	24	.37E-10
1.10	-1.7145065125	3.28295024	-8.358769	24	.20E-10
1.15	-1.5734499493	3.06658242	-7.733012	23	.55E-10
1.20	-1.4470542190	2.87562655	-7.188667	23	.31E-10
1.25	-1.3331716641	2.70593619	-6.711389	23	.18E-10
1.30	-1.2300529505	2.55420705	-6.289929	22	.59E-10
1.35	-1.1362590761	2.41777604	-5.915357	22	.37E-10
1.40	-1.0505956596	2.29447474	-5.580507	22	.23E-10
1.45	-.9720632084	2.18252085	-5.279568	22	.15E-10
1.50	-.8998190192	2.08043688	-5.007784	21	.56E-10
1.55	-.8331476616	1.98698822	-4.761230	21	.37E-10
1.60	-.7714378766	1.90113576	-4.536641	21	.26E-10
1.65	-.7141643202	1.82199898	-4.331279	21	.18E-10
1.70	-.6608730111	1.74882707	-4.142837	20	.74E-10
1.75	-.6111696343	1.68097610	-3.969353	20	.53E-10
1.80	-.5647100693	1.61789082	-3.809153	20	.38E-10
1.85	-.5211926635	1.55909000	-3.660799	20	.28E-10
1.90	-.4803518897	1.50415458	-3.523051	20	.21E-10
1.95	-.4419531044	1.45271805	-3.394831	20	.15E-10
2.00	-.4057881934	1.40445847	-3.275203	19	.74E-10
2.10	-.3394389265	1.31636732	-3.058537	19	.43E-10
2.20	-.2800451898	1.23797533	-2.867602	19	.26E-10
2.30	-.2265917168	1.16777028	-2.698132	19	.16E-10
2.40	-.1782507522	1.10453742	-2.546743	18	.71E-10
2.50	-.1343407465	1.04729003	-2.410720	18	.46E-10
2.60	-.0942954981	.99521856	-2.287861	18	.31E-10

Table 3 - Reduced 2nd Virial Coefficient Parameters for the 15.0 - 6.0 Potential Function (Cont'd)

T*	B*	B_1*	B_2*	J	Diff
2.70	-.0576407875	.94765267	-2.176360	18	.21E-10
2.80	-.0239764642	.90403268	-2.074727	18	.14E-10
2.90	.0070374404	.86388767	-1.981716	17	.76E-10
3.00	.0356915925	.82681865	-1.896282	17	.55E-10
3.10	.0622359593	.79248533	-1.817543	17	.40E-10
3.20	.0868866743	.76059574	-1.744745	17	.29E-10
3.30	.1098315591	.73089797	-1.677245	17	.22E-10
3.40	.1312345998	.70317357	-1.614486	17	.16E-10
3.50	.1512396006	.67723212	-1.555988	17	.12E-10
3.60	.1699731869	.65290695	-1.501334	16	.77E-10
3.70	.1875472877	.63005149	-1.450157	16	.60E-10
3.80	.2040612006	.60853638	-1.402138	16	.47E-10
3.90	.2196033185	.58824702	-1.356993	16	.37E-10
4.00	.2342525813	.56908148	-1.314473	16	.29E-10
4.10	.2480797015	.55094884	-1.274355	16	.23E-10
4.20	.2611482050	.53376773	-1.236441	16	.19E-10
4.30	.2735153175	.51746512	-1.200556	16	.15E-10
4.40	.2852327232	.50197526	-1.166541	16	.12E-10
4.50	.2963472168	.48723879	-1.134253	16	.10E-10
4.60	.3069012659	.47320202	-1.103565	15	.76E-10
4.70	.3169334972	.45981623	-1.074360	15	.63E-10
4.80	.3264791189	.44703714	-1.046533	15	.53E-10
4.90	.3355702892	.43482438	-1.019990	15	.44E-10
5.00	.3442364373	.42314110	-.994642	15	.37E-10
6.00	.4125210382	.32920192	-.792436	15	.79E-11
7.00	.4580706796	.26367058	-.653017	14	.24E-10
8.00	.4899737550	.21535947	-.551040	14	.83E-11
9.00	.5131085546	.17827810	-.473190	13	.41E-10
10.00	.5303162226	.14892798	-.411798	13	.19E-10
20.00	.5836395056	.02081324	-.144758	11	.42E-10
30.00	.5832528593	-.01968505	-.059206	10	.76E-10
40.00	.5746581534	-.03898815	-.017384	10	.15E-10
50.00	.5646735356	-.04999810	.007196	10	.44E-11
60.00	.5548990353	-.05694841	.023239	9	.50E-10
70.00	.5457467023	-.06162931	.034444	9	.23E-10
80.00	.5372899692	-.06492423	.042652	9	.12E-10
90.00	.5294976286	-.06731739	.048879	9	.67E-11
100.00	.5223085312	-.06909526	.053732	9	.40E-11
200.00	.4720320799	-.07437908	.072906	8	.76E-11
300.00	.4418916807	-.07398359	.077081	8	.13E-11
400.00	.4207691528	-.07275672	.078069	7	.31E-10

$B_1^* = T^* dB^*/dT^*$ $\qquad$ $B_2^* = T^{*2} d^2B^*/dT^{*2}$

B. The Derivatives B_1^* and B_2^*

Differentiation of [3] gives

$$B_1^* = a\{(m/n)\sum_j[(j-f_1)a^{j-f_1-1}\Gamma(f_1)]/(j-1)! - \sum_j[(j-f_2)a^{j-f_2-1}\Gamma(f_2)]/(j-1)!\} \quad [5]$$

and from [5], the second derivative is

$$B_2^* = -2B_1^* + a^2\{\sum_j[(j-f_2)(j-f_2-1)a^{j-f_2-2}\Gamma(f_2)]/(j-1)! - (m/n)\sum_j[(j-f_1)(j-f_1-1)a^{(j-f_1-2)}\Gamma(f_1)]/(j-1)!\} \quad [6]$$

Equations [5] and [6] have been used to calculate B_1^* and B_2^*, and the results are in columns 3 and 4, respectively of Tables 1, 2, and 3. The results for the 12.0-6.0 potential function compare favourably with those given by Hirschfelder et al(3) but are believed to be more accurate.

The computer program used to calculate these results is listed in Appendix A.

Extension of the analytical method to other more precise potential functions is dependent on the ability to integrate the expression in [2].

2. Numerical Results

A. The Reduced Second Virial Coefficient, B^*

For more complex and realistic potential functions, U(r), the integration of [2] cannot be carried out analytically. The numerical technique described in (4) has been used to determine B^*. This technique has been tested and results for the 12.0-6.0 potential function in Table 4 agree with those calculated from equation [3] and listed in Table 2, within the limits of precision of the two methods.

A listing of the computer program used to determine the results in Table 4 is provided in Appendix B.

B. The Derivatives B_1^* and B_2^*

Once B^* values have been determined the derivatives B_1^* and B_2^* can be obtained directly. A numerical differentiation technique in which B_1^* or B_2^* is the derivative at any value T^* of the Lagrangian interpolation polynomial of degree 2 relevant to three successive points, was used. The increment in T^* was varied by trial and error so that a smooth trend in B_2^* values was obtained. For each value of T^*, at which the values of B_1^* and B_2^* were desired, twenty values of B^* were used, centred about that value of T^*.

Table 4 lists values of B_1^* and B_2^* for the 12.0-6.0 potential, obtained numerically using the above method. These results can be compared with those calculated from equations [5] and [6] as given in Table 2. Agreement between the two sets of results is seen to be good.

Appendix C is a listing of the program used to carry out the numerical differentiation required to calculate the values of B_1^* and B_2^* in Table 4.

Table 4 - Reduced 2nd Virial Coefficient Parameters for the 12.0 - 6.0 Potential Function

T*	B*	B_1*	B_2*
.40	-13.7988347340	30.267080	-116.38405
.45	-10.7549741482	21.989481	-78.88383
.50	-8.7202054309	16.923691	-57.34379
.55	-7.2740854195	13.582155	-43.87763
.60	-6.1979710642	11.248850	-34.92000
.65	-5.3681917302	9.545510	-28.64550
.70	-4.7100373255	8.257115	-24.08345
.75	-4.1759282583	7.254013	-20.60161
.80	-3.7342253625	6.454140	-17.95200
.85	-3.3631194614	5.803406	-15.82275
.90	-3.0471142944	5.264919	-14.09400
.95	-2.7749102065	4.812761	-12.70265
1.00	-2.5380813464	4.428262	-11.54400
1.05	-2.3302211124	4.097666	-10.55506
1.10	-2.1463742035	3.810642	-9.71086
1.15	-1.9826492960	3.559293	-8.98275
1.20	-1.8359491362	3.337489	-8.34984
1.25	-1.7037784868	3.140408	-7.79453
1.30	-1.5841050765	2.964204	-7.30460
1.35	-1.4752573367	2.805783	-6.86900
1.40	-1.3758479738	2.662621	-6.47976
1.45	-1.2847161327	2.532646	-6.12931
1.50	-1.2008831619	2.414140	-5.81344
1.55	-1.1235182673	2.305668	-5.52635
1.60	-1.0519116807	2.206022	-5.26656
1.65	-.9854534122	2.114177	-5.02710
1.70	-.9236163909	2.029262	-4.80752
1.75	-.8659428370	1.950528	-4.60677
1.80	-.8120332758	1.877329	-4.42098
1.85	-.7615375218	1.809106	-4.24903
1.90	-.7141473736	1.745372	-4.08833
1.95	-.6695904798	1.685702	-3.93939
2.00	-.6276252928	1.629721	-3.80621
2.10	-.5506331885	1.527545	-3.55388
2.20	-.4817100511	1.436630	-3.33159
2.30	-.4196777438	1.355219	-3.13433
2.40	-.3635757791	1.281902	-2.95815
2.50	-.3126133820	1.215532	-2.79988
2.60	-.2661336222	1.155170	-2.65697
2.70	-.2235863521	1.100036	-2.52728
2.80	-.1845073659	1.049481	-2.40908
2.90	-.1485022922	1.002958	-2.30093
3.00	-.1152339760	.960003	-2.20163

Table 4 - Reduced 2nd Virial Coefficient Parameters for the 12.0 - 6.0 Potential Function (Cont'd)

T^*	B^*	B_1^*	B_2^*
3.10	-.0844124527	.920223	-2.11007
3.20	-.0557870459	.883278	-2.02547
3.30	-.0291399123	.848875	-1.94705
3.40	-.0042808604	.816761	-1.87411
3.50	.0189568897	.786715	-1.80614
3.60	.0407201899	.758543	-1.74270
3.70	.0611388358	.732076	-1.68325
3.80	.0803280015	.707163	-1.62746
3.90	.0983901810	.683672	-1.57503
4.00	.1154169153	.661483	-1.52560
4.10	.1314902040	.640492	-1.47903
4.20	.1466837110	.620605	-1.43501
4.30	.1610637939	.601735	-1.39341
4.40	.1746903839	.583808	-1.35389
4.50	.1876177416	.566755	-1.31645
4.60	.1998951095	.550512	-1.28081
4.70	.2115672672	.535024	-1.24687
4.80	.2226750585	.520239	-1.21461
4.90	.2332557603	.506110	-1.18381
5.00	.2433434958	.492595	-1.15444
6.00	.3229043708	.383972	-.91998
7.00	.3760884629	.308257	-.75815
8.00	.4134339521	.252480	-.64000
9.00	.4405978316	.209701	-.54979
10.00	.4608752809	.175867	-.48038
20.00	.5253741995	.028664	-.17072
30.00	.5269254516	-.017493	-.07211
40.00	.5185750133	-.039312	-.02420
50.00	.5083614230	-.051648	.00388
60.00	.4982126008	-.059362	.02205
70.00	.4886506870	-.064504	.03491
80.00	.4797900950	-.068082	.04400
90.00	.4716150432	-.070647	.05123
100.00	.4640694596	-.072524	.05651
200.00	.4114316782	-.077540	.07736
300.00	.3801278779	-.076525	.08147
400.00	.3583511795	-.074753	.08208

$B_1^* = T^* dB^*/dT^*$ $\qquad$ $B_2^* = T^{*2} d^2B^*/dT^{*2}$

exp-6 POTENTIAL FUNCTION

A. The Reduced Second Virial Coefficient, B^*

The numerical technique used above to test the calculation of B^* for the 12.0-6.0 potential function, has been used to determine B^* for the exp-6 potential function, which is given by

$$U(r) = \{\varepsilon/(1-6/\alpha)\}[6\ \exp\{\alpha(1-r/r_m)\}/\alpha-(r_m/r)^6] \qquad [7]$$

The parameters, r_m and α in [7] are, respectively, the value of r when U(r) is a minimum and the steepness of the exponential repulsion.

Results for the exp-6 potential function at various α values are listed in Tables 5 to 11. These results compare favourably with those given elsewhere(3) but are believed to be significantly more accurate (i.e. to at least 9 significant figures). This numerical integration technique should be applicable to any potential function U(r).

Table 5 - Derivatives of Reduced Second Virial Coefficient for α = 12.0

T^*	B^*	B_1^*	B_2^*
.40	-10.3480767778	22.756451	-87.93689
.45	-8.0623796302	16.489730	-59.46081
.50	-6.5381833667	12.662260	-43.14454
.55	-5.4572322100	10.142157	-32.96473
.60	-4.6543439960	8.385353	-26.18729
.65	-4.0362531749	7.104795	-21.44675
.70	-3.5467094875	6.137517	-17.98885
.75	-3.1499432753	5.385365	-15.38888
.80	-2.8222014161	4.786281	-13.38991
.85	-2.5471313776	4.299405	-11.79418
.90	-2.3131276317	3.896895	-10.51032
.95	-2.1117367157	3.559210	-9.44628
1.00	-1.9366613741	3.272284	-8.57756
1.05	-1.7831179363	3.025766	-7.83736
1.10	-1.6474095409	2.811883	-7.20497
1.15	-1.5266354475	2.624702	-6.65565
1.20	-1.4184885492	2.459620	-6.18564
1.25	-1.3211114752	2.313017	-5.77100
1.30	-1.2329924773	2.182011	-5.40583
1.35	-1.1528888715	2.064280	-5.08283
1.40	-1.0797699084	1.957935	-4.79045
1.45	-1.0127735689	1.861425	-4.52930
1.50	-.9511734895	1.773465	-4.29043
1.55	-.8943533555	1.692980	-4.07693
1.60	-.8417868719	1.619067	-3.89639
1.65	-.7930219459	1.550964	-3.70830
1.70	-.7476680847	1.488016	-3.55368
1.75	-.7053862734	1.429666	-3.40608
1.80	-.6658807810	1.375433	-3.25532
1.85	-.6288924817	1.324898	-3.13077
1.90	-.5941933727	1.277700	-3.00456
1.95	-.5615820479	1.233518	-2.90820
2.00	-.5308799382	1.192078	-2.80933
2.10	-.4745849296	1.116462	-2.60977
2.20	-.4242290589	1.049203	-2.44561
2.30	-.3789424624	.988993	-2.29989
2.40	-.3380163511	.934783	-2.16989
2.50	-.3008674507	.885722	-2.05274
2.60	-.2670114536	.841111	-1.94747
2.70	-.2360429276	.800372	-1.85196
2.80	-.2076199242	.763023	-1.76463
2.90	-.1814520499	.728658	-1.68480

Table 5 - Derivatives of Reduced Second Virial Coefficient for α = 12.0 (Cont'd)

T^*	B^*	B_1^*	B_2^*
3.00	-.1572911282	.696934	-1.61147
3.10	-.1349238167	.667558	-1.54374
3.20	-.1141657202	.640278	-1.48141
3.30	-.0948566562	.614878	-1.42409
3.40	-.0768568196	.591171	-1.37006
3.50	-.0600436525	.568992	-1.31976
3.60	-.0443092735	.548198	-1.27302
3.70	-.0295583522	.528663	-1.22923
3.80	-.0157063427	.510277	-1.18809
3.90	-.0026780061	.492941	-1.14931
4.00	.0095938303	.476567	-1.11275
4.10	.0211693214	.461078	-1.07844
4.20	.0321024932	.446403	-1.04582
4.30	.0424420003	.432430	-1.01543
4.40	.0522317744	.419253	-.98684
4.50	.0615115805	.406671	-.95940
4.60	.0703174971	.394687	-.93278
4.70	.0786823316	.383261	-.90759
4.80	.0866359804	.372353	-.88391
4.90	.0942057430	.361930	-.86117
5.00	.1014165966	.351960	-.83925
6.00	.1580252389	.271831	-.66543
7.00	.1954983065	.215981	-.54671
8.00	.2215235026	.174840	-.45987
9.00	.2402182589	.143289	-.39357
10.00	.2539754233	.118338	-.34126
20.00	.2937026608	.009935	-.11301
30.00	.2903576289	-.023809	-.04086
40.00	.2811063051	-.039569	-.00568
50.00	.2712495477	-.048335	.01487
60.00	.2619255725	-.053703	.02819
70.00	.2533669994	-.057191	.03741
80.00	.2455668836	-.059541	.04410
90.00	.2384546528	-.061161	.04907
100.00	.2319487834	-.062289	.05296
200.00	.1876668771	-.064128	.06641
300.00	.1619303218	-.062711	.06663
400.00	.1440490184	-.061625	.06509

$B_1^* = T^* dB^*/dT^*$ $\qquad$ $B_2^* = T^{*2} d^2B^*/dT^{*2}$

Table 6 - Derivatives of Reduced Second Virial Coefficient for $\alpha = 12.5$

T^*	B^*	B_1^*	B_2^*
.40	-10.0516469185	22.146702	-85.54257
.45	-7.8270270601	16.050443	-57.84984
.50	-6.3433347525	12.326682	-41.98330
.55	-5.2909673823	9.874606	-32.07478
.60	-4.5092172902	8.165051	-25.48856
.65	-3.9073362042	6.918814	-20.87618
.70	-3.4305868119	5.977376	-17.51303
.75	-3.0441583546	5.245254	-14.98259
.80	-2.7249324739	4.662077	-13.02930
.85	-2.4569923346	4.188093	-11.48278
.90	-2.2290407593	3.796212	-10.23340
.95	-2.0328482948	3.467422	-9.20643
1.00	-1.8622841424	3.188038	-8.35008
1.05	-1.7126907828	2.947983	-7.62985
1.10	-1.5804686306	2.739697	-7.01528
1.15	-1.4627931139	2.557404	-6.48468
1.20	-1.3574175879	2.396625	-6.02445
1.25	-1.2625332676	2.253835	-5.62302
1.30	-1.1766678807	2.126231	-5.26632
1.35	-1.0986111390	2.011553	-4.94873
1.40	-1.0273591223	1.907961	-4.66740
1.45	-.9620722154	1.813946	-4.41337
1.50	-.9020429064	1.728255	-4.18491
1.55	-.8466708551	1.649844	-3.97800
1.60	-.7954433899	1.577835	-3.78637
1.65	-.7479201069	1.511482	-3.61359
1.70	-.7037205980	1.450150	-3.45691
1.75	-.6625145935	1.393296	-3.30751
1.80	-.6240139838	1.340451	-3.17546
1.85	-.5879663137	1.291209	-3.05080
1.90	-.5541494448	1.245216	-2.93385
1.95	-.5223671466	1.202163	-2.82668
2.00	-.4924454343	1.161779	-2.72866
2.10	-.4375811948	1.088088	-2.54470
2.20	-.3885050945	1.022537	-2.38446
2.30	-.3443695262	.963854	-2.24220
2.40	-.3044838116	.911017	-2.11526
2.50	-.2682795611	.863195	-2.00121
2.60	-.2352848116	.819709	-1.89918
2.70	-.2051044544	.779997	-1.80561
2.80	-.1774052383	.743587	-1.72100
2.90	-.1519041498	.710085	-1.64114

Table 6 - Derivatives of Reduced Second Virial Coefficient for α = 12.5 (Cont'd)

T^*	B^*	B_1^*	B_2^*
3.00	-.1283593133	.679156	-1.57017
3.10	-.1065627990	.650515	-1.50505
3.20	-.0863348860	.623917	-1.44378
3.30	-.0675194494	.599152	-1.38787
3.40	-.0499802231	.576035	-1.33537
3.50	-.0335977501	.554408	-1.28668
3.60	-.0182668763	.534131	-1.24062
3.70	-.0038946805	.515082	-1.19774
3.80	.0096012480	.497151	-1.15812
3.90	.0222942488	.480245	-1.12041
4.00	.0342497996	.464276	-1.08475
4.10	.0455265381	.449169	-1.05154
4.20	.0561771283	.434857	-1.01979
4.30	.0662489987	.421277	-.98963
4.40	.0757849741	.408376	-.96139
4.50	.0848238181	.396103	-.93439
4.60	.0934007010	.384413	-.90872
4.70	.1015476044	.373267	-.88463
4.80	.1092936725	.362626	-.86134
4.90	.1166655181	.352458	-.83907
5.00	.1236874904	.342732	-.81802
6.00	.1787977073	.264550	-.64928
7.00	.2152549547	.210041	-.53326
8.00	.2405539740	.169877	-.44842
9.00	.2587088608	.139067	-.38366
10.00	.2720523675	.114695	-.33260
20.00	.3102037840	.008684	-.11048
30.00	.3064961542	-.024412	-.03949
40.00	.2971114725	-.039915	-.00475
50.00	.2871913994	-.048566	.01502
60.00	.2778306402	-.053881	.02881
70.00	.2692465987	-.057346	.03675
80.00	.2614262036	-.059691	.04480
90.00	.2542961998	-.061314	.04859
100.00	.2477738369	-.062449	.05249
200.00	.2033594700	-.064304	.06717
300.00	.1776318847	-.062335	.06927
400.00	.1599982909	-.060186	.06718

$B_1^* = T^* dB^*/dT^*$ $\qquad$ $B_2^* = T^{*2} d^2B^*/dT^{*2}$

Table 7 - Derivatives of Reduced Second Virial Coefficient for $\alpha = 13.0$

T^*	B^*	B_1^*	B_2^*
.40	-9.7870210827	21.600808	-83.38871
.45	-7.6170580843	15.657628	-56.40930
.50	-6.1695799098	12.026773	-40.94219
.55	-5.1427492487	9.635663	-31.29077
.60	-4.3798711138	7.968430	-24.86547
.65	-3.7924532787	6.752920	-20.36478
.70	-3.3271135875	5.834603	-17.08702
.75	-2.9498997163	5.120395	-14.61809
.80	-2.6382612864	4.551439	-12.71780
.85	-2.3766711416	4.088976	-11.20887
.90	-2.1541077716	3.706591	-9.98376
.95	-1.9625419104	3.385746	-8.98596
1.00	-1.7959914597	3.113093	-8.14752
1.05	-1.6499115572	2.878809	-7.44591
1.10	-1.5207894602	2.675516	-6.85100
1.15	-1.4058685759	2.497584	-6.33491
1.20	-1.3029562059	2.340642	-5.88321
1.25	-1.2102869039	2.201254	-5.48582
1.30	-1.1264236014	2.076684	-5.14386
1.35	-1.0501848942	1.964726	-4.83222
1.40	-.9805907768	1.863588	-4.55523
1.45	-.9168216009	1.771795	-4.30852
1.50	-.8581866520	1.688127	-4.08792
1.55	-.8040998205	1.611564	-3.89072
1.60	-.7540605699	1.541249	-3.69798
1.65	-.7076389058	1.476455	-3.52452
1.70	-.6644633994	1.416562	-3.38027
1.75	-.6242115674	1.361040	-3.23764
1.80	-.5866020837	1.309432	-3.10951
1.85	-.5513884309	1.261340	-2.97675
1.90	-.5183536889	1.216421	-2.86918
1.95	-.4873062324	1.174372	-2.76560
2.00	-.4580761555	1.134928	-2.66933
2.10	-.4044796780	1.062950	-2.48428
2.20	-.3565372226	.998[illegible]	-2.32809
2.30	-.3134209741	.941595	-2.18971
2.40	-.2744563558	.889978	-2.06561
2.50	-.2390882093	.843259	-1.95445
2.60	-.2068555430	.800775	-1.85433
2.70	-.1773724211	.761974	-1.76337
2.80	-.1503133203	.726400	-1.68034
2.90	-.1254017824	.693665	-1.60385

Table 7 - Derivatives of Reduced Second Virial Coefficient for α = 13.0 (Cont'd)

T^*	B^*	B_1^*	B_2^*
3.00	-.1024015287	.663443	-1.53451
3.10	-.0811094357	.635456	-1.47021
3.20	-.0613499332	.609465	-1.41101
3.30	-.0429704990	.585262	-1.35629
3.40	-.0258380088	.562671	-1.30474
3.50	-.0098357575	.541535	-1.25698
3.60	.0051389879	.521718	-1.21275
3.70	.0191770110	.503099	-1.17104
3.80	.0323588278	.485574	-1.13177
3.90	.0447560927	.469049	-1.09455
4.00	.0564327798	.453440	-1.06074
4.10	.0674461810	.438674	-1.02717
4.20	.0778477522	.424683	-.99686
4.30	.0876838345	.411408	-.96735
4.40	.0969962712	.398796	-.93989
4.50	.1058229382	.386798	-.91333
4.60	.1141982002	.375370	-.88834
4.70	.1221533069	.364473	-.86396
4.80	.1297167356	.354070	-.84129
4.90	.1369144907	.344128	-.81975
5.00	.1437703644	.334618	-.79925
6.00	.1975647338	.258165	-.63355
7.00	.2331324385	.204847	-.52049
8.00	.2577974218	.165551	-.43774
9.00	.2754823912	.135398	-.37455
10.00	.2884669979	.111540	-.32471
20.00	.3252717090	.007643	-.10662
30.00	.3212686041	-.024889	-.03762
40.00	.3117809866	-.040176	-.00385
50.00	.3018140471	-.048735	.01596
60.00	.2924260669	-.054016	.02883
70.00	.2838221227	-.057473	.03776
80.00	.2759844076	-.059825	.04427
90.00	.2688377332	-.061464	.04918
100.00	.2622985603	-.062620	.05294
200.00	.2176961777	-.064695	.06699
300.00	.1917806985	-.062864	.06918
400.00	.1739891549	-.060731	.06901

$B_1^* = T^* dB^*/dT^*$ $\qquad$ $B_2^* = T^{*2} d^2B^*/dT^{*2}$

Table 8 - Derivatives of Reduced Second Virial Coefficient for $\alpha = 13.5$

T^*	B^*	B_1^*	B_2^*
.40	-9.5486596135	21.107706	-81.46522
.45	-7.4280456449	15.302944	-55.10066
.50	-6.0132358270	11.756344	-40.00119
.55	-5.0094237171	9.420363	-30.57034
.60	-4.2635450182	7.791377	-24.29641
.65	-3.6891475089	6.603619	-19.90410
.70	-3.2340737113	5.706174	-16.70472
.75	-2.8651466708	5.008133	-14.29324
.80	-2.5603287765	4.452005	-12.43070
.85	-2.3044445112	3.999929	-10.95882
.90	-2.0867210170	3.626104	-9.76552
.95	-1.8993095263	3.312418	-8.78669
1.00	-1.7363619686	3.045829	-7.97501
1.05	-1.5934349872	2.816741	-7.28384
1.10	-1.4670940614	2.617945	-6.69833
1.15	-1.3546438118	2.443938	-6.19366
1.20	-1.2539401036	2.290450	-5.75350
1.25	-1.1632564948	2.154122	-5.37102
1.30	-1.0811875921	2.032280	-5.03074
1.35	1.0065779740	1.922770	-4.72886
1.40	-.9384691436	1.823838	-4.45790
1.45	-.8760594058	1.734044	-4.21755
1.50	-.8186731473	1.652194	-3.99645
1.55	-.7657370499	1.577293	-3.79929
1.60	-.7167614823	1.508500	-3.61836
1.65	-.6713258035	1.445107	-3.45363
1.70	-.6290666518	1.386508	-3.30156
1.75	-.5896685376	1.332183	-3.16394
1.80	-.5528562277	1.281685	-3.03572
1.85	-.5183885363	1.234628	-2.91389
1.90	-.4860532293	1.190672	-2.80523
1.95	-.4556628155	1.149525	-2.70071
2.00	-.4270510503	1.110925	-2.60865
2.10	-.3745876674	1.040486	-2.43223
2.20	-.3276581217	.977821	-2.27893
2.30	-.2854523551	.921716	-2.14432
2.40	-.2473102348	.871195	-2.02194
2.50	-.2126884686	.825466	-1.91370
2.60	-.1811359031	.783879	-1.81602
2.70	-.1522748264	.745898	-1.72614
2.80	-.1257866425	.711073	-1.64573
2.90	-.1014007684	.679027	-1.57049

Table 8 - Derivatives of Reduced Second Virial Coefficient for $\alpha = 13.5$ (Cont'd)

T^*	B^*	B_1^*	B_2^*
3.00	-.0788859410	.649440	-1.50267
3.10	-.0580433435	.622039	-1.43922
3.20	-.0387011240	.596591	-1.38131
3.30	-.0207099874	.572895	-1.32743
3.40	-.0039396235	.550775	-1.27757
3.50	.0117242084	.530079	-1.23033
3.60	.0263820735	.510674	-1.18683
3.70	.0401228413	.492443	-1.14606
3.80	.0530253318	.475281	-1.10794
3.90	.0651596908	.459098	-1.07173
4.00	.0765885468	.443812	-1.03754
4.10	.0873679872	.429350	-1.00559
4.20	.0975483869	.415648	-.97534
4.30	.1071751139	.402647	-.94652
4.40	.1162891337	.390294	-.91952
4.50	.1249275275	.378543	-.89402
4.60	.1331239400	.367349	-.86931
4.70	.1409089662	.356675	-.84610
4.80	.1483104869	.346485	-.82404
4.90	.1553539623	.336747	-.80290
5.00	.1620626869	.327431	-.78255
6.00	.2146933401	.252529	-.62109
7.00	.2494771329	.200280	-.51013
8.00	.2735855001	.161761	-.42896
9.00	.2908596222	.132198	-.36705
10.00	.3035318236	.108800	-.31810
20.00	.3391904967	.006798	-.10508
30.00	.3349572467	-.025232	-.03679
40.00	.3254008277	-.040330	-.00315
50.00	.3154090627	-.048813	.01627
60.00	.3060098511	-.054066	.02881
70.00	.2973984498	-.057522	.03798
80.00	.2895535483	-.059886	.04640
90.00	.2823987071	-.061543	.04657
100.00	.2758500095	-.062721	.05499
200.00	.2310986788	-.065045	.06717
300.00	.2050042618	-.063399	.06927
400.00	.1870399393	-.061397	.06878

$B_1^* = T^* dB^*/dT^*$ $\qquad$ $B_2^* = T^{*2} d^2B^*/dT^{*2}$

Table 9 - Derivatives of Reduced Second Virial Coefficient for $\alpha = 14.0$

T^*	B^*	B_1^*	B_2^*
.40	-9.3323328707	20.658965	-79.69206
.45	-7.2566088044	14.980558	-53.90970
.50	-5.8714895217	11.510668	-39.14778
.55	-4.8885817846	9.224909	-29.92256
.60	-4.1581308119	7.630745	-23.78497
.65	-3.5955427795	6.468241	-19.48991
.70	-3.1497752289	5.589782	-16.35673
.75	-2.7883567778	4.906438	-14.00484
.80	-2.4897161986	4.361967	-12.17371
.85	-2.2389976619	3.919329	-10.73196
.90	-2.0256542746	3.553276	-9.57061
.95	-1.8420012361	3.246089	-8.60687
1.00	-1.6823121840	2.985004	-7.82749
1.05	-1.5422359072	2.760631	-7.13992
1.10	-1.4184088718	2.565914	-6.56056
1.15	-1.3081912333	2.395466	-6.07368
1.20	-1.2094829038	2.245109	-5.64199
1.25	-1.1205928087	2.111557	-5.25923
1.30	-1.0401442700	1.992188	-4.92414
1.35	-.9670054152	1.884896	-4.63628
1.40	-.9002372371	1.787963	-4.36902
1.45	-.8390543059	1.699980	-4.12980
1.50	-.7827946864	1.619777	-3.91916
1.55	-.7308966447	1.546380	-3.72254
1.60	-.6828804239	1.478966	-3.55718
1.65	-.6383338506	1.416842	-3.39519
1.70	-.5969008654	1.359413	-3.23576
1.75	-.5582723083	1.306173	-3.09982
1.80	-.5221784595	1.256681	-2.97181
1.85	-.4883829573	1.210559	-2.86552
1.90	-.4566778066	1.167477	-2.74283
1.95	-.4268792558	1.127145	-2.64202
2.00	-.3988243720	1.089310	-2.54932
2.10	-.3473812587	1.020262	-2.38337
2.20	-.3013634673	.958832	-2.23380
2.30	-.2599769926	.903830	-2.10095
2.40	-.2225747559	.854301	-1.98236
2.50	-.1886241883	.809467	-1.87584
2.60	-.1576830248	.768693	-1.77962
2.70	-.1293809826	.731452	-1.69228
2.80	-.1034057223	.697305	-1.61271
2.90	-.0794919666	.665881	-1.53971

Table 9 - Derivatives of Reduced Second Virial Coefficient for $\alpha = 14.0$ (Cont'd).

T^*	B^*	B_1^*	B_2^*
3.00	-.0574129808	.636868	-1.47285
3.10	-.0369738362	.609998	-1.41134
3.20	-.0180060375	.585042	-1.35417
3.30	-.0003632022	.561803	-1.30156
3.40	.0160824406	.540109	-1.25271
3.50	.0314429077	.519812	-1.20675
3.60	.0458168085	.500779	-1.16414
3.70	.0592912861	.482897	-1.12415
3.80	.0719436302	.466064	-1.08664
3.90	.0838426263	.450191	-1.05120
4.00	.0950496894	.435197	-1.01754
4.10	.1056198207	.421011	-.98640
4.20	.1156024205	.407570	-.95673
4.30	.1250419797	.394816	-.92852
4.40	.1339786722	.382698	-.90165
4.50	.1424488634	.371169	-.87738
4.60	.1504855488	.360188	-.85236
4.70	.1581187331	.349715	-.83027
4.80	.1653757603	.339718	-.80903
4.90	.1722815998	.330163	-.78734
5.00	.1788590978	.321023	-.76799
6.00	.2304539814	.247523	-.60832
7.00	.2645428762	.196240	-.49978
8.00	.2881600168	.158425	-.42032
9.00	.3050733113	.129395	-.35960
10.00	.3174725902	.106414	-.31173
20.00	.3521583302	.006125	-.10184
30.00	.3477540893	-.025451	-.03537
40.00	.3581614860	-.040379	-.00275
50.00	.3281670970	-.048795	.01645
60.00	.3187735759	-.054026	.02896
70.00	.3101685088	-.057483	.03769
80.00	.3023281483	-.059859	.04407
90.00	.2951754001	-.061536	.04885
100.00	.2886263340	-.062737	.05261
200.00	.2437870362	-.065306	.06672
300.00	.2175493369	-.063848	.06922
400.00	.1994358859	-.061985	.06934

$B_1^* = T^* dB^*/dT^*$ $\qquad$ $B_2^* = T^{*2} d^2B^*/dT^{*2}$

Table 10 - Derivatives of Reduced Second Virial Coefficient for $\alpha = 14.5$

T^*	B^*	B_1^*	B_2^*
.40	-9.1347395639	20.248004	-78.07916
.45	-7.1001084196	14.685579	-52.82222
.50	-5.7421451542	11.286057	-38.36195
.55	-4.7783430432	9.046337	-29.32926
.60	-4.0619830388	7.484078	-23.31315
.65	-3.5101749512	6.344700	-19.10530
.70	-3.0728979187	5.483618	-16.04305
.75	-2.7183266840	4.813721	-13.72629
.80	-2.4253169071	4.279912	-11.93773
.85	-2.1793052459	3.845901	-10.52520
.90	-1.9699514628	3.486953	-9.38271
.95	-1.7897206564	3.185703	-8.44592
1.00	-1.6329976920	2.929647	-7.66246
1.05	-1.4955155415	2.709578	-7.00124
1.10	-1.3739755042	2.518585	-6.43811
1.15	-1.2657884422	2.351387	-5.95473
1.20	-1.1688944741	2.203888	-5.53205
1.25	-1.0816348014	2.072866	-5.16395
1.30	-1.0026589448	1.955754	-4.83635
1.35	-.9308565127	1.850485	-4.54544
1.40	-.8653062721	1.755375	-4.28882
1.45	-.8052376237	1.669043	-4.05590
1.50	-.7500011022	1.590342	-3.84597
1.55	-.6990455319	1.518317	-3.65512
1.60	-.6519001548	1.452161	-3.48074
1.65	-.6081605130	1.391193	-3.32260
1.70	-.5674771994	1.334831	-3.17872
1.75	-.5295468199	1.282577	-3.04335
1.80	-.4941046759	1.234001	-2.92029
1.85	-.4609187988	1.188732	-2.80693
1.90	-.4297850533	1.146445	-2.69918
1.95	-.4005230922	1.106856	-2.60089
2.00	-.3729729973	1.069717	-2.50865
2.10	-.3224544825	1.001937	-2.34181
2.20	-.2772626740	.941633	-2.19471
2.30	-.2366181721	.887635	-2.06443
2.40	-.1998857736	.839008	-1.94705
2.50	-.1665426627	.794990	-1.84182
2.60	-.1361546569	.754956	-1.74841
2.70	-.1083582283	.718389	-1.66198
2.80	-.0828467247	.684859	-1.58379
2.90	-.0593596918	.654002	-1.51246

Table 10 Derivatives of Reduced Second Virial Coefficient for $\alpha = 14.5$ (Cont'd)

T^*	B^*	B_1^*	B_2^*
3.00	-.0376745101	.625511	-1.44776
3.10	-.0175997838	.599124	-1.38636
3.20	.0010299326	.574616	-1.33036
3.30	.0183583759	.551793	-1.27815
3.40	.0345110104	.530487	-1.22988
3.50	.0495978331	.510552	-1.18531
3.60	.0637156775	.491859	-1.14276
3.70	.0769501189	.474295	-1.10362
3.80	.0893770581	.457761	-1.06750
3.90	.1010640455	.442169	-1.03256
4.00	.1120713943	.427441	-.99994
4.10	.1224531204	.413506	-.96871
4.20	.1322577395	.400302	-.93950
4.30	.1415289465	.387773	-.91196
4.40	.1503061973	.375869	-.88587
4.50	.1586252077	.364543	-.86098
4.60	.1665183842	.353754	-.83756
4.70	.1740151967	.343466	-.81517
4.80	.1811425015	.333643	-.79394
4.90	.1879248237	.324256	-.77349
5.00	.1943846025	.315276	-.75396
6.00	.2450522916	.243052	-.59840
7.00	.2785218838	.192648	-.49161
8.00	.3017033838	.155474	-.41334
9.00	.3182984192	.126930	-.35369
10.00	.3304584204	.104329	-.30660
20.00	.3643198599	.005603	-.10098
30.00	.3597966356	-.025560	-.03499
40.00	.3501972609	-.040334	-.00275
50.00	.3402207388	-.048688	.01627
60.00	.3308488440	-.053900	.02971
70.00	.3222633262	-.057358	.03675
80.00	.3144389158	-.059746	.04480
90.00	.3072983767	-.061442	.04859
100.00	.3007580805	-.062665	.05499
200.00	.2558947909	-.065469	.06637
300.00	.2295549365	-.064192	.06927
400.00	.2113228446	-.062466	.06878

$B_1^* = T^* dB^*/dT^*$ $\qquad$ $B_2^* = T^{*2} d^2B^*/dT^{*2}$

Table 11 - Derivatives of Reduced Second Virial Coefficient for $\alpha = 15.0$

T^*	B^*	B_1^*	B_2^*
.40	-8.9532543982	19.869594	-76.56649
.45	-6.9564457616	14.414202	-51.81590
.50	-5.6234566103	11.079575	-37.63618
.55	-4.6772123293	8.882289	-28.78439
.60	-3.9737934888	7.349420	-22.88095
.65	-3.4318801103	6.231335	-18.75451
.70	-3.0023924151	5.386246	-15.74897
.75	-2.6541000541	4.728719	-13.47599
.80	-2.3662515570	4.204714	-11.72563
.85	-2.1245526477	3.778634	-10.34175
.90	-1.9188531215	3.426215	-9.21417
.95	-1.7417558688	3.130420	-8.29999
1.00	-1.5877479643	2.878981	-7.53747
1.05	-1.4526397133	2.662866	-6.87804
1.10	-1.3331919554	2.475291	-6.32458
1.15	-1.2268621070	2.311076	-5.84883
1.20	-1.1316271913	2.166200	-5.43317
1.25	-1.0458580279	2.037500	-5.07172
1.30	-.9682281735	1.922458	-4.75512
1.35	-.8976469397	1.819044	-4.46769
1.40	-.8332093937	1.725606	-4.21711
1.45	-.7741585342	1.640787	-3.99313
1.50	-.7198563268	1.563464	-3.78415
1.55	-.6697612736	1.492696	-3.59640
1.60	-.6234108629	1.427693	-3.41637
1.65	-.5804077065	1.367784	-3.26587
1.70	-.5404084918	1.312400	-3.12016
1.75	-.5031151058	1.261051	-2.99263
1.80	-.4682674491	1.213315	-2.87460
1.85	-.4356375760	1.168827	-2.75428
1.90	-.4050248852	1.127268	-2.65257
1.95	-.3762521468	1.088360	-2.55646
2.00	-.3491622018	1.051859	-2.47932
2.10	-.2994863095	.985241	-2.30044
2.20	-.2550469971	.925966	-2.15598
2.30	-.2150782291	.872889	-2.02793
2.40	-.1789556662	.825088	-1.91366
2.50	-.1461654129	.781816	-1.81098
2.60	-.1162806787	.742460	-1.71810
2.70	-.0889441116	.706511	-1.63377
2.80	-.0638542592	.673545	-1.55704
2.90	-.0407550751	.643207	-1.48714

Table 11 - Derivatives of Reduced Second Virial Coefficient for α = 15.0 (Cont'd)

T^*	B^*	B_1^*	B_2^*
3.00	-.0194277013	.615194	-1.42222
3.10	.0003160294	.589249	-1.36281
3.20	.0186387765	.565151	-1.30834
3.30	.0356818593	.542709	-1.25718
3.40	.0515686353	.521758	-1.20994
3.50	.0664072566	.502154	-1.16540
3.60	.0802929349	.483771	-1.12429
3.70	.0933098139	.466499	-1.08582
3.80	.1055325260	.450239	-1.04981
3.90	.1170274944	.434905	-1.01545
4.00	.1278540267	.420420	-.98314
4.10	.1380652391	.406715	-.95320
4.20	.1477088399	.393728	-.92409
4.30	.1568277979	.381405	-.89755
4.40	.1654609136	.369696	-.87212
4.50	.1736433103	.358556	-.84802
4.60	.1814068574	.347944	-.82433
4.70	.1887805364	.337824	-.80210
4.80	.1957907593	.328162	-.78080
4.90	.2024616456	.318928	-.76093
5.00	.2088152638	.310093	-.74237
6.00	.2586486610	.239038	-.58773
7.00	.2915636320	.189441	-.48293
8.00	.3143570558	.152853	-.40622
9.00	.3306702645	.124754	-.34757
10.00	.3426197913	.102501	-.30130
20.00	.3757845026	.005209	-.09822
30.00	.3711873901	-.025573	-.03386
40.00	.3616070652	-.040204	-.00219
50.00	.3516666127	-.048501	.01649
60.00	.3423306484	-.053696	.02871
70.00	.3337766485	-.057155	.03724
80.00	.3259786003	-.059556	.04347
90.00	.3188595649	-.061268	.04822
100.00	.3123364845	-.062513	.05194
200.00	.2675096576	-.065537	.06612
300.00	.2411078632	-.064432	.06889
400.00	.2227878368	-.062838	.06924

$B_1^* = T^* dB^*/dT^*$ $\qquad$ $B_2^* = T^{*2} d^2B^*/dT^{*2}$

B. The Derivatives B_1^* and B_2^*

The numerical method described above and tested for the 12.0-6.0 potential function was used to obtain B_1^* and B_2^* from the B^* values for the exp-6 potential function at α values ranging from 12.0 to 15.0.B^* values determined at small and variable increments in T^* over the range of T^* resulted in accurate values of B_1^* and B_2^*. Tests of the increments required to obtain convergence of the B_2^* results were carried out throughout the range of T^* values used. The values of B_1^* and B_2^* listed in Tables 5 to 11 are believed to be respectively accurate to at least seven and five significant figures.

Values of B_1^* have been determined previously(5) by an indirect method and the results are included in Table 12 for comparison. On the basis of the B_1^* values calculated here for the 12.0-6.0 potential, it is believed that the results calculated here are more accurate by at least two orders of magnitude.

There are no values in the literature available for comparison with the B_2^* values listed in Tables 5 to 11. However, it is believed these values are accurate to at least five significant figures. Comparison with the values of B_2^* calculated by the numerical method for the 12.0-6.0 potential function supports this contention.

Table 12 - Comparison of B_1^* Values at $\alpha = 12.0$

T^*	B^*	B_1^* Calculated	B_1^* (5)
.40	-10.3480767778	22.756451	22.7565
.45	-8.0623796302	16.489730	16.4897
.50	-6.5381833667	12.662260	12.6622
.55	-5.4572322100	10.142157	10.1421
.60	-4.6543439960	8.385353	8.3853
.65	-4.0362531749	7.104795	7.1048
.70	-3.5467094875	6.137517	6.1375
.75	-3.1499432753	5.385365	5.3853
.80	-2.8222014161	4.786281	4.7863
.85	-2.5471313776	4.299405	4.2994
.90	-2.3131276317	3.896895	3.8968
.95	-2.1117367157	3.559210	3.5592
1.00	-1.9366613741	3.272284	3.2723
1.05	-1.7831179363	3.025766	3.0257
1.10	-1.6474095409	2.811883	2.8118
1.15	-1.5266354475	2.624702	2.6247
1.20	-1.4184885492	2.459620	2.4596
1.25	-1.3211114752	2.313017	2.3130
1.30	-1.2329924773	2.182011	2.1820
1.35	-1.1528888715	2.064280	2.0643
1.40	-1.0797699084	1.957935	1.9579
1.45	-1.0127735689	1.861425	1.8614
1.50	-.9511734895	1.773465	1.7734
1.55	-.8943533555	1.692980	1.6930
1.60	-.8417868719	1.619067	1.6190
1.65	-.7930219459	1.550964	1.5509
1.70	-.7476680847	1.488016	1.4880
1.75	-.7053862734	1.429666	1.4296
1.80	-.6658807810	1.375433	1.3754
1.85	-.6288924817	1.324898	1.3249
1.90	-.5941933727	1.277700	1.2777
1.95	-.5615820479	1.233518	1.2335
2.00	-.5308799382	1.192078	1.1920
2.10	-.4745849296	1.116462	1.1164
2.20	-.4242290589	1.049203	1.0492
2.30	-.3789424624	.988993	.9890
2.40	-.3380163511	.934783	.9348
2.50	-.3008674507	.885722	.8857
2.60	-.2670114536	.841111	.8411
2.70	-.2360429276	.800372	.8003
2.80	-.2076199242	.763023	.7630
2.90	-.1814520499	.728658	.7286

Table 12 - Comparison of B_1^* Values at $\alpha = 12.0$ (Cont'd)

T^*	B^*	B_1^* Calculated	B_1^* (5)
3.00	-.1572911282	.696934	.6969
3.10	-.1349238167	.667558	.6675
3.20	-.1141657202	.640278	.6402
3.30	-.0948566562	.614878	.6149
3.40	-.0768568196	.591171	.5911
3.50	-.0600436525	.568992	.5690
3.60	-.0443092735	.548198	.5482
3.70	-.0295583522	.528663	.5286
3.80	-.0157063427	.510277	.5102
3.90	-.0026780061	.492941	.4929
4.00	.0095938303	.476567	.4765
4.10	.0211693214	.461078	.4610
4.20	.0321024932	.446403	.4464
4.30	.0424420003	.432480	.4324
4.40	.0522317744	.419253	.4192
4.50	.0615115805	.406671	.4066
4.60	.0703174971	.394687	.3947
4.70	.0786823316	.383261	.3832
4.80	.0866359804	.372353	.3723
4.90	.0942057430	.361930	.3619
5.00	.1014165966	.351960	.3519
6.00	.1580252389	.271831	.2718
7.00	.1954983065	.215981	.2159
8.00	.2215235026	.174840	.1748
9.00	.2402182589	.143289	.1433
10.00	.2539754233	.118338	.1183
20.00	.2937026608	.009935	.0099
30.00	.2903576289	-.023809	-.0238
40.00	.2811063051	-.039569	-.0396
50.00	.2712495477	-.048335	-.0484
60.00	.2619255725	-.053703	-.0537
70.00	.2533669994	-.057191	-.0572
80.00	.2455668836	-.059541	-.0596
90.00	.2384546528	-.061161	-.0612
100.00	.2319487834	-.062289	-.0623
200.00	.1876668771	-.064128	-.0641
300.00	.1619303218	-.062711	-.0627
400.00	.1440490184	-.061625	-.0616

$$B_1^* = T^* dB^*/dT^*$$

CONCLUSION

The numerical method for determining B^* has been shown to give accurate results, which in turn will permit calculation of potential function parameters. The latter are required to predict detonation parameters and fume composition used to classify explosives.

Additionally, reliable numerical results for the derivatives, B_1^* and B_2^* have been obtained. The first values of B_2^* have been reported for the exp-6 potential function, thus permitting estimation of thermodynamic functions characteristic of that potential function.

Extension of these methods to other potential functions, or equations of state, are required, both to further test the methods and to provide more realistic data in the prediction of explosive properties.

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APPENDIX A

```
      PROGRAM ANAGAM
$DEBUG
$NOTRUNCATE
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION FAC(50)
      DATA ONE,FAC,TWO,THREE/3*1.0D0,48*0.0D0,2.0D0,3.0D0/
      OPEN(2,FILE='BSTAR',STATUS='UNKNOWN')
   75 WRITE(*,1000)
 1000 FORMAT(' ENTER N AND M - FREE FORMAT - N < 0.0 TO STOP',/)
      READ(*,*) PN,PM
      IF (PN.LT.0.0) GO TO 500
      NSKIP = 1
      NINK = 1
  100 WRITE(*,1001)
 1001 FORMAT(' ENTER STARTING VALUE , INCREMENT AND END VALUE OF TSTAR ,
     1 - TSTAR < 0.0 TO STOP',/)
      READ(*,*) TSTAR,DTSTAR,TSTARM
      IF (TSTAR.LT.0.0) GO TO 75
      IF (NSKIP.GT.1) GO TO 150
      WRITE(*,200) PN,PM
      WRITE(2,200) PN,PM
  200 FORMAT(///,' RESULTS FOR THE ',F5.2,' -',F5.2,' POTENTIAL FUNCTION
     1',//)
      WRITE(*,115)
      WRITE(2,115)
  115 FORMAT('    TSTAR   ',     BSTAR   ',        TdBdT    ',
     1'      T2d2BdT2 ,'         J',      DIFF',/)
      PNM = PN - PM
      PPNM = PM/PNM
      FNM = (PN/PNM)*(PN/PM)**PPNM
  150 BSTAR = 0.0D0
      TDBDT = 0.0D0
      TD2BDT2 = 0.0D0
      STORE = 0.0D0
      A = FNM/TSTAR
      A2 = A**2
      M = 50
      DO 20 J = 1,M
      JP1 = J + 1
      FJ = FLOAT(J)
      FAC(J + 2) = JP1*FAC(JP1)
      F1 = (FJ*PM - THREE)/PN
      F1J = FJ - F1
      F2 = (PN + (FJ - ONE)*PM - THREE)/PN
      F2J = FJ - F2
```

```
      TERM1 = GAMMA(F1)*A**F1J*PM/PN
      TERM11 = F1J*GAMMA(F1)*A**(F1J - ONE)*PM/PN
      TERM12 = (F1J - ONE)*F1J*GAMMA(F1)*A**(F1J - TWO)*PM/PN
      TERM2 = GAMMA(F2)*A**F2J
      TERM21 = F2J*GAMMA(F2)*A**(F2J - ONE)
      TERM22 = (F2J - ONE)*F2J*GAMMA(F2)*A**(F2J - TWO)
      BSTAR = BSTAR + (TERM2 - TERM1)/FAC(J)
      DIFF = BSTAR-STORE
      IF (ABS(DIFF).GT.0.8D-10) GO TO 25
      BSTAR = STORE
      GO TO 30
   25 STORE = BSTAR
      TDBDT = TDBDT + (TERM11 - TERM21)/FAC(J)
      TD2BDT2 = TD2BDT2 + (TERM22 - TERM12)/FAC(J)
   20 CONTINUE
   30 TDBDT = TDBDT*A
      TD2BDT2 = TD2BDT2*A2
      TD2BDT2 = TD2BDT2 - TWO*TDBDT
      WRITE(*,400) TSTAR,BSTAR,TDBDT,TD2BDT2,J,DIFF
      WRITE(2,400) TSTAR,BSTAR,TDBDT,TD2BDT2,J,DIFF
  400 FORMAT(G10.5,F15.10,2F15.8,4X,I2,E10.2)
      IF (NINK.EQ.42) WRITE(2,88)
   88 FORMAT('1')
   10 CONTINUE
      TSTAR = TSTAR + DTSTAR
      NINK = NINK + 1
      IF (TSTAR.LE.TSTARM) GO TO 150
      NSKIP = NSKIP + 1
      GO TO 100
  500 STOP
      END
      FUNCTION GAMMA(XX)
      REAL*8 COF(6),STP,HALF,ONE,FPF,X,TMP,SER,GAMLN,GAMMA,XX
      DATA COF,STP/76.18009173D0,-86.50532033D0,24.01409822D0,
     1-1.231739516D0,.120858003D-2,-.536382D-5,2.50662827465D0/
      DATA HALF,ONE,FPF/0.50D0,1.0D0,5.5D0/
      X = XX - ONE
      TMP = X + FPF
      TMP = (X + HALF)*DLOG(TMP) - TMP
      SER = ONE
      DO 11 J = 1,6
      X = X + ONE
      SER = SER + COF(J)/X
   11 CONTINUE
      GAMLN = TMP + DLOG(STP*SER)
      GAMMA = DEXP(GAMLN)
      RETURN
      END
```

APPENDIX B

```
      PROGRAM GAUSS
$DEBUG
$NOTRUNCATE
C
C
C
C
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION TABLE(20),A(10),B(10),FINT(10)
C
C              UNIT NUMBERS:  KW - SCREEN OUTPUT
C                             KF - OUTPUT TO FILE 'GAIT'
C                             KI - INPUT FILE
C                             KO - OUTPUT FILE B* vs T*
C
      DATA A,B,FINT/30*0.0D0/
      KW = 6
      KF = 8
      KI = 7
      KO = 9
      OPEN(KF,FILE='GAIT',STATUS='UNKNOWN')
      OPEN(KI,FILE='GAITIN',STATUS='UNKNOWN')
      OPEN(KO,FILE= BSTS',STATUS='UNKNOWN')
C
C
C
  200 READ (KI,*) KLI,IOFLAG,NOPT
      IF (KLI.LE.0) STOP
C
C
      READ(KI,*) (A(I),I=1,NOPT)
      DO 10 I = 1,NOPT
      IF (I.EQ.1) GO TO 10
      IM1 = I - 1
      B(IM1) = A(I)
   10 CONTINUE
C
      READ(KI,*) ALPHAS,DALPHA,ALPHAE
      READ(KI,*) TSS,DTSS,TSSE,NEWT
      ALPHA = ALPHAS
  300 TS = TSS
      DTS = DTSS
      TSE = TSSE
      NEWSET = NEWT
C
```

```
C
  400 KPRT = 1
      IF (IOFLAG.EQ.1) KPRT = 2
      BS = 0.0D0
C
      DO 100 I = 1,NOPT-1
      KL = KLI
      FINT(I) = 0.0D0
      CALL GAUSSQ(A(I),B(I),KL,TABLE,KPRT,KF,KW,TS,ALPHA,NUMSD)
C
      DO 170 J = 1, 20
         IF (NUMSD.LT.12) THEN
            KOPT = 1
         ELSE
            KOPT = 0
         ENDIF
         IF (KOPT.NE.1) GO TO 171
         CALL AITKEN(TABLE,KL,KPRT,KF,KW,NUMSD)
         KL = KL - 2
         IF (KL.LT.3) GO TO 171
  170    CONTINUE
C
  171 FINT(I) = TABLE(KL)
      BS = BS + FINT(I)
  100 CONTINUE
C
      WRITE (*,*)
      WRITE(KW,169) TS,BS,ALPHA
      IF (TS.EQ.TSS) THEN
                     WRITE(KO,249) TS,BS,ALPHA
      ELSE
                     WRITE(KO,250) TS,BS
      ENDIF
  249 FORMAT(F10.6,F20.10,10X,F4.1)
  250 FORMAT(F10.6,F20.10)
      IF (KPRT.GE.2) WRITE(KF,169) TS,BS,ALPHA
  169 FORMAT(//,' TS =',F10.6,' BS =',F14.10,' ALPHA =',F5.1,//)
      TS = TS + DTS
      IF (TS.LE.TSE) GO TO 400
      IF (NEWSET.EQ.1) THEN
         READ(KI,*) TSI,DTS,TSE,NEWSET
         TS = TSI
         GO TO 400
      ELSE
         ALPHA = ALPHA + DALPHA
      ENDIF
      IF (ALPHA.LE.ALPHAE) GO TO 300
      GO TO 200
C
      END
```

```
      SUBROUTINE GAUSSQ(A,B,KL,TABLE,KPRT,KF,KW,TSTAR,ALPHA,NUMSD)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
C  ITERATIVE GAUSS QUADRATURE.  FUNCTION NUMBER NFCT IS INTEGRATED FROM
C  A TO B PRODUCING KL LINES IN TABLE USING
C  1, 2, 4, 8, 16, ..., 2**(KL-1) SUBINTERVALS.
C
C  IF KPRT IS 1 THE TABLE IS WRITTEN ON UNIT KW.
C  IF KPRT IS 2 THE TABLE IS ALSO WRITTEN ON UNIT KF.
C
C  IN THE TABLE WHICH IS WRITTEN:
C
C  N         IS THE NUMBER OF SUBINTERVALS USED,
C  GAUSS     IS THE GAUSS QUADRATURE APPROXIMATION TO THE INTEGRAL,
C  TOTAL NF  IS THE TOTAL NUMBER OF FUNCTION EVALUATIONS DONE SO FAR,
C  EST S.D.  IS A CONSERVATIVE ESTIMATE OF THE NUMBER OF SIGNIFICANT
C            DIGITS WHICH ARE CORRECT IN THAT LINE
C
C  THE EXTERNAL FUNCTION CALLED IS F(X,NFCT) FOR THE FUNCTION BEING
C  INTEGRATED.
C
      DIMENSION TABLE(20)
C
C             SET EPS TO THE SIZE OF THE ROUNDING ERRORS FOR A GIVEN
C             MACHINE.  EPS = 1.0E-7 FOR 32 BIT MACHINES (SINGLE
C             PRECISION) OR 1.0E-16 (DOUBLE PRECISION).
C
      EPS = 1.0E-7
C
C             CHECK FOR ERRORS.
C
      IF (KL.LT.1) THEN
          WRITE (KW,110) KL
  110     FORMAT(/' ERROR IN GAUSSQ.  KL=',I5,'.  IT SHOULD BE AT ',
     *           'LEAST 1.')
          DO 120 J = 1, 20
  120        TABLE(J) = -3.1E+31
          RETURN
      ENDIF
C
C             DO GAUSS QUADRATURE FOR THE INTEGRAL OF F(X) FROM A TO B.
C
      NLINES = KL
      SQRT3 = DSQRT(3.0D0)
      NSUBS = 1
      NFUNCT = 0
C
      IF (KPRT.GE.1) THEN
          WRITE (KW,130) NLINES
          IF (KPRT.GE.2) WRITE (KF,130) NLINES
  130     FORMAT(/' GAUSS INTEGRATION OF EXP - 6 FUNCTION .  THERE',
     *           ' ARE',I3,' LINES IN THE TABLE.')
          WRITE (KW,140) A,B
```

```
      IF (KPRT.GE.2) WRITE (KF,140) A,B
140   FORMAT(/' THE LIMITS OF INTEGRATION ARE:'/3X,D7.2,
     *       '  TO  ',D7.2/)
      ENDIF
C
      DO 180 JLINE = 1, NLINES
C
C           THE KTH SUBINTERVAL IS (AK,BK).  THE GAUSS APPROXIMATION
C           FOR THE INTEGRAL IS:  XH*(F(XM-XR) + F(XM+XR)), WHERE
C           XH = (BK-AK)/2,   XM = (AK+BK)/2,   XR = XH/(2*SQRT(3)),
C           AK = A + (K-1)*(B-A)/NSUBS,   BK = A + K*(B-A)/NSUBS.
C
      XH = (B-A)/NSUBS
      XH2 = XH/2.0
      XR = XH2/SQRT3
      START1 = A - XH2 - XR
      START2 = A - XH2 + XR
      SUM = 0.0
C
      DO 150 K = 1, NSUBS
C
150      SUM = SUM + F(START1+K*XH,TSTAR,ALPHA) + F(START2
     *+K*XH,TSTAR,ALPHA)
      SUM = SUM*XH2
      NFUNCT = NFUNCT + 2*NSUBS
      IF (KPRT.GE.1) THEN
          IF (JLINE.LE.1) THEN
              WRITE (KW,160) NSUBS,SUM,NFUNCT
              IF (KPRT.GE.2) WRITE (KF,160) NSUBS,SUM,NFUNCT
160           FORMAT(' N =',I6,'  GAUSS=',D23.16,'     TOTAL NF=',I5)
          ELSE
              RELERR = EPS
              IF (SUM.NE.0.0) RELERR = DABS(TABLE(JLINE-1)-SUM)
     *                                 / DABS(SUM)
              IF (SUM.EQ.0.0 .AND. TABLE(JLINE-1).NE.0.0) RELERR =
     *            DABS(TABLE(JLINE-1)-SUM) / DABS(TABLE(JLINE-1))
              IF (RELERR.LE.0.0) RELERR = EPS
              NUMSD = -DLOG10(RELERR)
              IF (NUMSD.LT.0) NUMSD = 0
              WRITE (KW,170) NSUBS,SUM,NFUNCT,NUMSD
              IF (KPRT.GE.2) WRITE (KF,170) NSUBS,SUM,NFUNCT,NUMSD
170           FORMAT(' N =',I6,'  GAUSS=',D23.16,'     TOTAL NF=',I5,
     *                       ' EST S.D.=',I3)
          ENDIF
      ENDIF
      NSUBS = 2*NSUBS
      TABLE(JLINE) = SUM
180   CONTINUE
    TABLE(KL) = TABLE(NLINES)
    RETURN
    END
```

```
      SUBROUTINE AITKEN(TABLE,KL,KPRT,KF,KW,NUMSD)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
C  AITKEN EXTRAPOLATION.  THE VALUES TABLE(1) TO TABLE(KL) ARE USED FOR
C  THE EXTRAPOLATION AND THE RESULTS ARE RETURNED IN TABLE(1) TO
C  TABLE(KL-2).  KL MUST BE AT LEAST 3.
C
C  IF KPRT IS 1 THEN THE KL-2 VALUES ARE WRITTEN ON UNIT KW.
C  IF KPRT IS 2 THE TABLE IS ALSO WRITTEN ON UNIT KF.
C
C  IN THE TABLE WHICH IS WRITTEN:
C
C  LINE      IS THE LINE NUMBER,
C  AITKEN    IS THE AITKEN EXTRAPOLATION APPROXIMATION TO THE INTEGRAL,
C            USING 3 VALUES FROM THE PREVIOUS COLUMN.  FOR EXAMPLE,
C            LINE 1 OF AN AITKEN COLUMN USES LINES 1-3 OF THE PREVIOUS
C            COLUMN, LINE 4 USES LINES 4-6, ETC.
C  EST S.D. IS A CONSERVATIVE ESTIMATE OF THE NUMBER OF SIGNIFICANT
C            DIGITS WHICH ARE CORRECT IN THAT LINE
C
      DIMENSION TABLE(20)
C
C             SET EPS TO THE SIZE OF THE ROUNDING ERRORS FOR A GIVEN
C             MACHINE.  EPS = 1.0E-7 FOR 32 BIT MACHINES (SINGLE
C             PRECISION) OR 1.0E-16 (DOUBLE PRECISION).
C
      EPS = 1.0E-7
C
      IF (KL.LT.3) THEN
          WRITE (KW,110) KL
  110     FORMAT(//' ERROR IN AITKEN.  KL=',I5,' IS LESS THAN 3.'/)
          RETURN
      ENDIF
C
      IF (KPRT.GE.1) THEN
          KLM2 = KL - 2
          WRITE (KW,120) KLM2
          IF (KPRT.GE.2) THEN
              IF (KLM2.GT.1) THEN
                  WRITE (KF,120) KLM2
  120             FORMAT(/' AITKEN COLUMN.',I4,' ENTRIES.'/)
              ELSE
                  WRITE (KF,130) KLM2
  130             FORMAT(/' AITKEN COLUMN.',I4,' ENTRY.'/)
              ENDIF
          ENDIF
      ENDIF
C
```

```
      KLM1 = KL - 1
      DO 160 JLINE = 2, KLM1
         TOP = (TABLE(JLINE+1) - TABLE(JLINE))**2
         BOT = TABLE(JLINE+1) - 2.0*TABLE(JLINE) + TABLE(JLINE-1)
         IF (BOT.EQ.0.0) THEN
             TABLE(JLINE-1) = TABLE(JLINE+1)
         ELSE
             TABLE(JLINE-1) = TABLE(JLINE+1) - TOP/BOT
         ENDIF
         IF (KPRT.GE.1) THEN
             JLM1 = JLINE - 1
             IF (JLINE.LE.2) THEN
                 WRITE (KW,140) JLM1,TABLE(JLM1)
                 IF (KPRT.GE.2) WRITE (KF,140) JLM1,TABLE(JLM1)
  140            FORMAT(' LINE',I3,'  AITKEN=',D23.16)
             ELSE
                 RELERR = EPS
                 IF (TABLE(JLM1).NE.0.0) RELERR = DABS(TABLE(JLM1-1) -
     *                                    TABLE(JLM1))/DABS(TABLE(JLM1))
                 IF (TABLE(JLM1).EQ.0.0 .AND. TABLE(JLM1-1).NE.0.0)
     *               RELERR = DABS(TABLE(JLM1-1)-TABLE(JLM1)) /
     *                        DABS(TABLE(JLM1-1))
                 IF (RELERR.LE.0.0) RELERR = EPS
                 NUMSD = -DLOG10(RELERR)
                 IF (NUMSD.LT.0) NUMSD = 0
                 WRITE (KW,150) JLM1,TABLE(JLM1),NUMSD
                 IF (KPRT.GE.2) WRITE (KF,150) JLM1,TABLE(JLM1),NUMSD
  150            FORMAT(' LINE',I3,'  AITKEN=',D23.16,
     *                        '  EST S.D.=',I3)
             ENDIF
         ENDIF
  160    CONTINUE
      RETURN
      END
      FUNCTION F(X,TSTAR,ALPHA)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      FX = DEXP(ALPHA*(1.0D0 - X))
      AA = 6.0D0/ALPHA
      TSA = TSTAR*(1.0D0 - AA)
      TSA = 1.0D0/TSA
      F1 = 1.0D0/X**4 - X**3*FX
      F2 = DEXP(-TSA*(AA*FX - 1.0D0/X**6))
      F = F1*F2
      F = -6.0D0*TSA*F
      RETURN
C
      CLOSE(KF,STATUS='KEEP')
      CLOSE(KO,STATUS='KEEP')
      END
```

APPENDIX C

```
      PROGRAM MAIN
$DEBUG
$NOTRUNCATE
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION TS(900),BS(900),DYDT(900),Y(900),BSLJBZ(900),
     1 TBPSLJ(900),T2B2PSL(900),D2YDT2(900)
      CHARACTER*10 DATAFIL,RESOUT
 2000 WRITE(*,3)
    3 FORMAT('1',' INPUT THE NAME OF THE OUTPUT FILE',////)
      READ(*,4) RESOUT
    4 FORMAT(A10)
      IF (RESOUT.EQ.'END') THEN
         WRITE(3,9)
    9    FORMAT(//,'      B1* = T*dB*/dT*     B2* = T*2d2B*/dT*2')
         STOP
      ELSE
         OPEN(3,FILE=RESOUT,STATUS='UNKNOWN')
      ENDIF
      KFILE = 0
 1000 WRITE(*,1)
    1 FORMAT('1',' INPUT THE NAME OF THE DATA FILE ,////)
      READ(*,2) DATAFIL
    2 FORMAT(A10)
      IF (DATAFIL.EQ.'NEW ALPHA') GO TO 2000
      IF (DATAFIL.EQ.'NONE') STOP
      KFILE = KFILE + 1
      OPEN(2,FILE=DATAFIL,STATUS='OLD')
      READ(2,*) NPTS,BZ,PN,PM
      DO 10 K = 1 ,NPTS
      IF (K.EQ.1) THEN
      READ(2,500) TS(K),BS(K),ALPHA
  500 FORMAT(F10.6,F20.10,10X,F4.1)
      ELSE
      READ(2,501) TS(K),BS(K)
  501 FORMAT(F10.6,F20.10)
      ENDIF
      CALL NMPOT(PN,PM,TS(K),BSLJ,TBPSLJ(K),T2B2PSL(K))
      BSLJBZ(K) = BSLJ - BZ
      BSBZ = BS(K) - BZ
      Y(K) = BSBZ/BSLJBZ(K)
   10 CONTINUE
```

```
      CALL DDGT3(TS,Y,DYDT,NPTS,IER)
      CALL DDGT3(TS,DYDT,D2YDT2,NPTS,IER)
      IF (KFILE.GT.1) GO TO 110
      WRITE(*,90) ALPHA
      WRITE(3,91) ALPHA
   90 FORMAT('1',' DERIVATIVES OF REDUCED SECOND VIRIAL COEFFICIENT FOR
     1ALPHA =',F5.1,//)
   91 FORMAT(' DERIVATIVES OF REDUCED SECOND VIRIAL COEFFICIENT FOR ALPH
     1A =',F5.1,//)
      WRITE(*,101)
      WRITE(3,100)
  100 FORMAT('     T*   ','          B*  ','            B1*     ',
     1'       B2*      ',/)
  101 FORMAT('       T*   ','            B*  ','            B1*    ',
     1'       B2*      ',/)
  110 DO 20 K = 2 , NPTS
      KP1 = K + 1
      TS2 = TS(K)**2
      TDBDT = TS(K)*DYDT(KP1)*BSLJBZ(K) + Y(K)*TBPSLJ(K)
      T2D2BDT = Y(K)*T2B2PSL(K) + BSLJBZ(K)*TS2*D2YDT2(KP1)
     1 + 2.0D0*TS(K)*DYDT(KP1)*TBPSLJ(K)
      TM = 0.05D0
      BOA = 0.3D0
      DO 21 L = 1 ,85
      BOA = BOA + TM
      IF (BOA.GT.1.99) TM = 0.1D0
      IF (BOA.GT.4.99) TM = 1.0D0
      IF (BOA.GT.9.99) TM = 10.0D0
      IF (BOA.GT.99.) TM = 100.0D0
      IF (TS(K).GT.BOA-.1D-6.AND.TS(K).LT.BOA+.1D-6) WRITE(3,201)
     1 TS(K),BS(K),TDBDT,T2D2BDT
  200 FORMAT(F11.6,3X,F14.10,3X,F10.6,3X,F10.5)
  201 FORMAT(F7.2,3X,F14.10,3X,F10.6,3X,F10.5)
   21 CONTINUE
      WRITE(*,200) TS(K),BS(K),TDBDT,T2D2BDT
   20 CONTINUE
      GO TO 1000
      END
```

```
      SUBROUTINE DDGT3(X,Y,Z,NDIM,IER)
      DIMENSION X(900),Y(900),Z(900)
      DOUBLE PRECISION X,Y,Z,DY1,DY2,DY3,A,B
      IER = -1
      IF (NDIM - 3) 8,1,1
    1 A = X(1)
      B = Y(1)
      I = 2
      DY2 = X(2) - A
      IF (DY2) 2,9,2
    2 DY2 = (Y(2) - B)/DY2
      DO 6 I = 3 , NDIM
      A = X(I) - A
      IF (A) 3,9,3
    3 A = (Y(I) - B)/A
      B = X(I) - X(I - 1)
      IF (B) 4,9,4
    4 DY1 = DY2
      DY2 = (Y(I) - Y(I - 1))/B
      DY3 = A
      A = X(I - 1)
      B = Y(I - 1)
      IF (I - 3) 5,5,6
    5 Z(I) = DY1 + DY3 - DY2
    6 Z(I) = DY1 + DY2 - DY3
      IER = 0
      I = NDIM
    7 Z(I) = DY2 + DY3 - DY1
    8 RETURN
    9 IER = I
      I = I - 1
      IF (I - 2) 8,8,7
      END
```

```
      SUBROUTINE NMPOT(PN,PM,TSTAR,BSTAR,TDBDT,TD2BDT2)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION FAC(50)
      DATA ONE,FAC,TWO,THREE/3*1.0D0,48*0.0D0,2.0D0,3.0D0/
      PNM = PN - PM
      PPNM = PM/PNM
      FNM = (PN/PNM)*(PN/PM)**PPNM
  150 BSTAR = 0.0D0
      TDBDT = 0.0D0
      TD2BDT2 = 0.0D0
      STORE = 0.0D0
      A = FNM/TSTAR
      A2 = A**2
      M = 50
      DO 20 J = 1 , M
      FJ = FLOAT(J)
      JP1 = J + 1
      FAC(J + 2) = JP1*FAC(JP1)
      F1 = (FJ*PM - THREE)/PN
      F1J = FJ - F1
      F1J1 = F1J - ONE
      F1J2 = F1J - TWO
      F2 = (PN + (FJ - ONE)*PM - THREE)/PN
      F2J = FJ - F2
      F2J1 = F2J - ONE
      F2J2 = F2J - TWO
      G1MN = GAMMA(F1)*PM/PN
      G2 = GAMMA(F2)
      F1G1 = F1J*G1MN
      F2G2 = F2J*G2
      TERM1 = G1MN*A**F1J
      TERM11 = F1G1*A**F1J1
      TERM12 = F1J1*F1G1*A**F1J2
      TERM2 = G2*A**F2J
      TERM21 = F2G2*A**F2J1
      TERM22 = F2J1*F2G2*A**F2J2
      BSTAR = BSTAR + (TERM2 - TERM1)/FAC(J)
      IF (DABS(BSTAR-STORE).GT..8D-10) GO TO 25
      BSTAR = STORE
      GO TO 30
   25 STORE = BSTAR
      TDBDT = TDBDT + (TERM11 - TERM21)/FAC(J)
      TD2BDT2 = TD2BDT2 + (TERM22 - TERM12)/FAC(J)
   20 CONTINUE
   30 TDBDT = TDBDT*A
      TD2BDT2 = TD2BDT2*A2
      TD2BDT2 = TD2BDT2 - TWO*TDBDT
      END
```

```
      FUNCTION GAMMA(XX)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION COF(6)
      DATA COF,STP/76.18009173D0,-86.50532033D0,24.01409822D0,
     1-1.231739516D0,0.120858003D-2,-0.536382D-5,2.50662827465D0/
      DATA HALF,ONE,FPF/0.50D0,1.0D0,5.5D0/
      X = XX - ONE
      TMP = X + FPF
      TMP = (X + HALF)*DLOG(TMP) - TMP
      SER = ONE
      DO 11 J = 1 , 6
      X = X + ONE
      SER = SER + COF(J)/X
   11 CONTINUE
      GAMLN = TMP + DLOG(STP*SER)
      GAMMA = DEXP(GAMLN)
      RETURN
      END
```